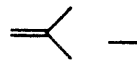
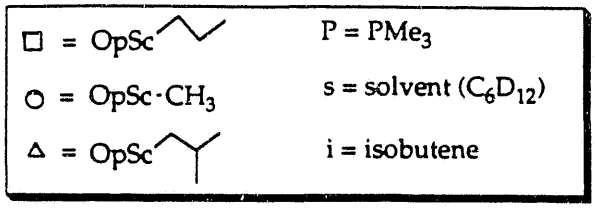
ORGANOMETALLICS

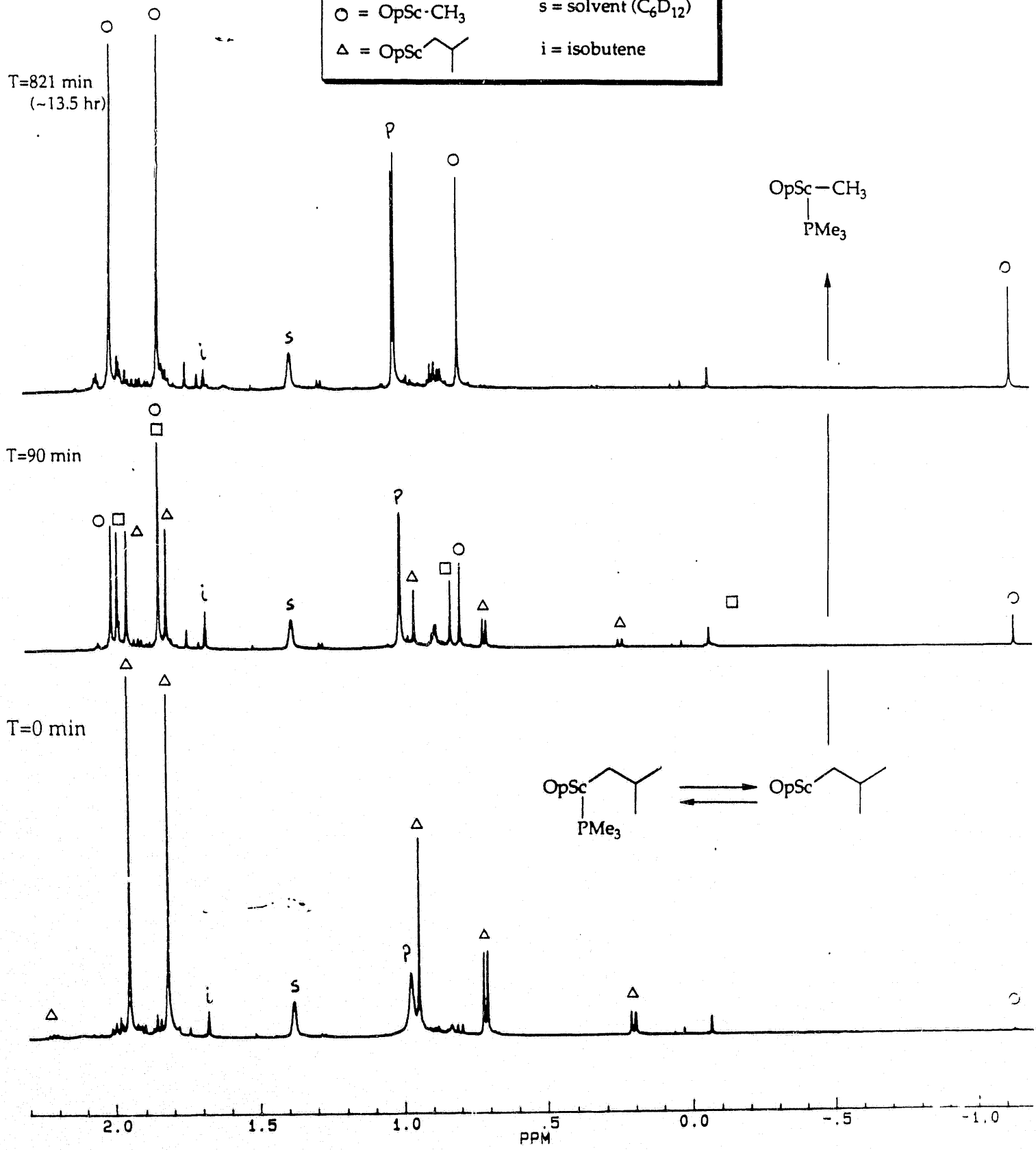
Supporting Information for *Organometallics*, **1994**, 13(4), 1147-1154, DOI: 10.1021/om00016a018

HAJELA
1147-1154

L-1154-m1

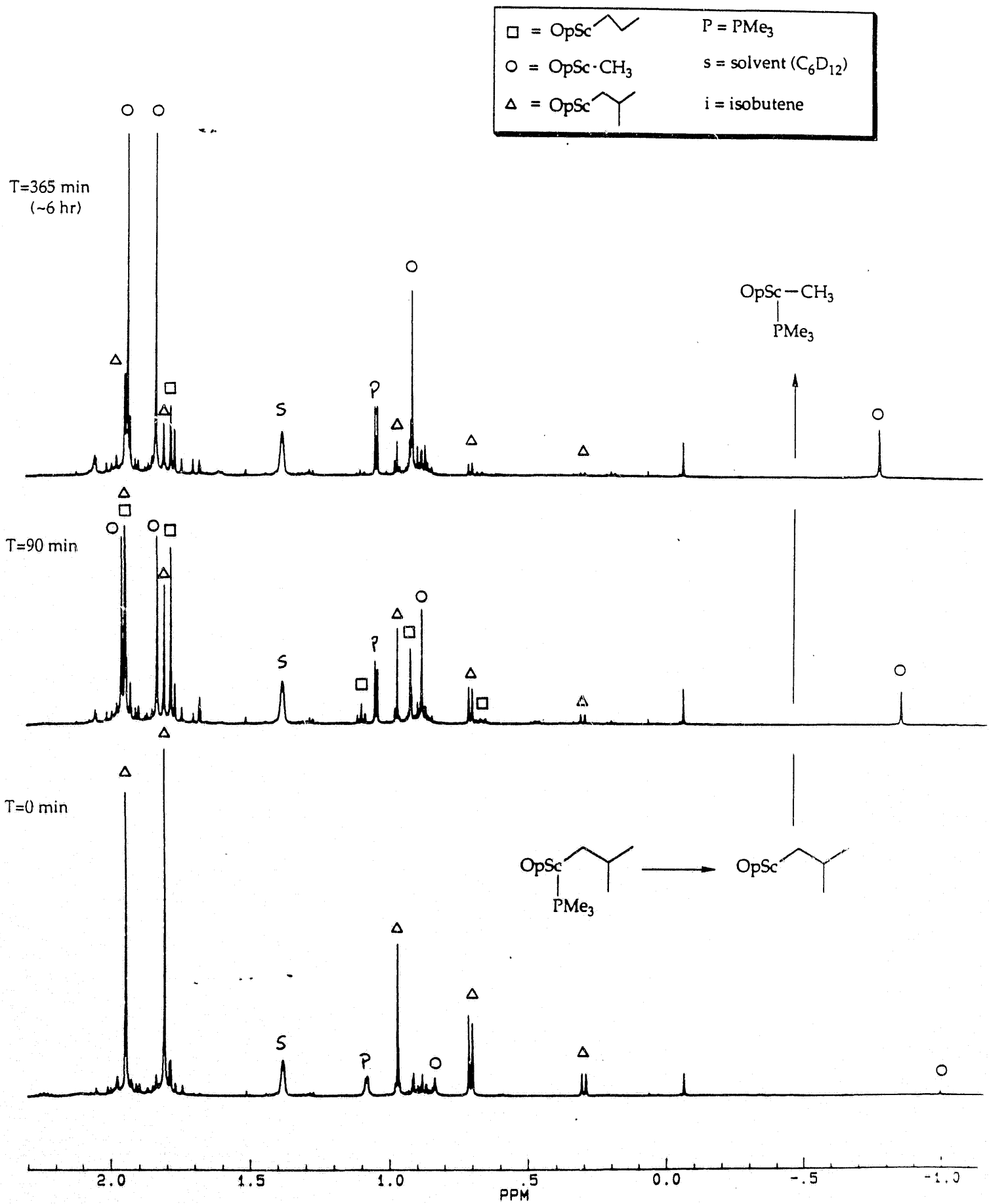
Selected Spectra From Kinetic Run: $OpScH(PMe_3)$ +  ⟶ $OpScCH_3(PMe_3)$





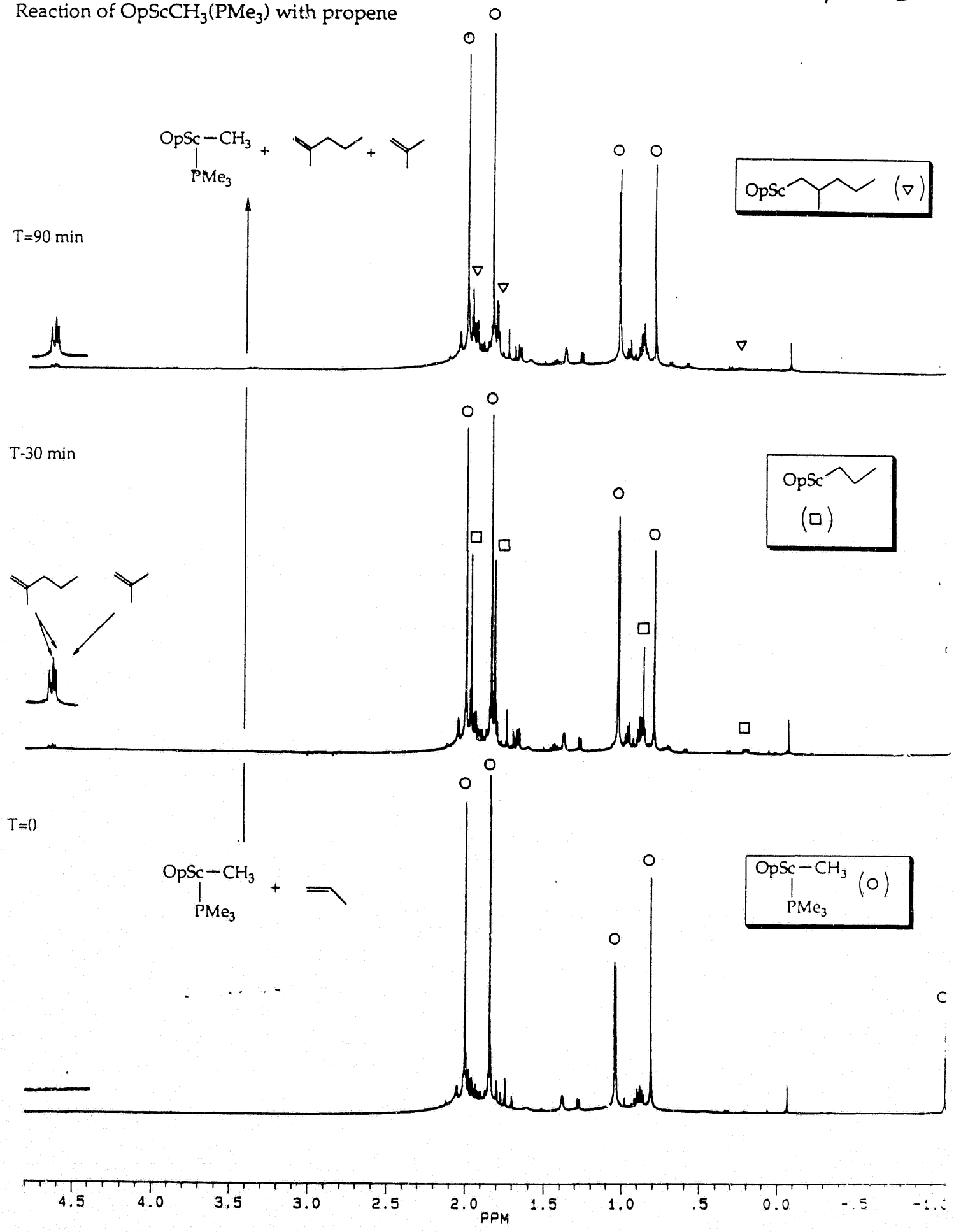
L-1154-m2

Rearrangement of OpSc(isobutyl) After Pumping Off PMe_3

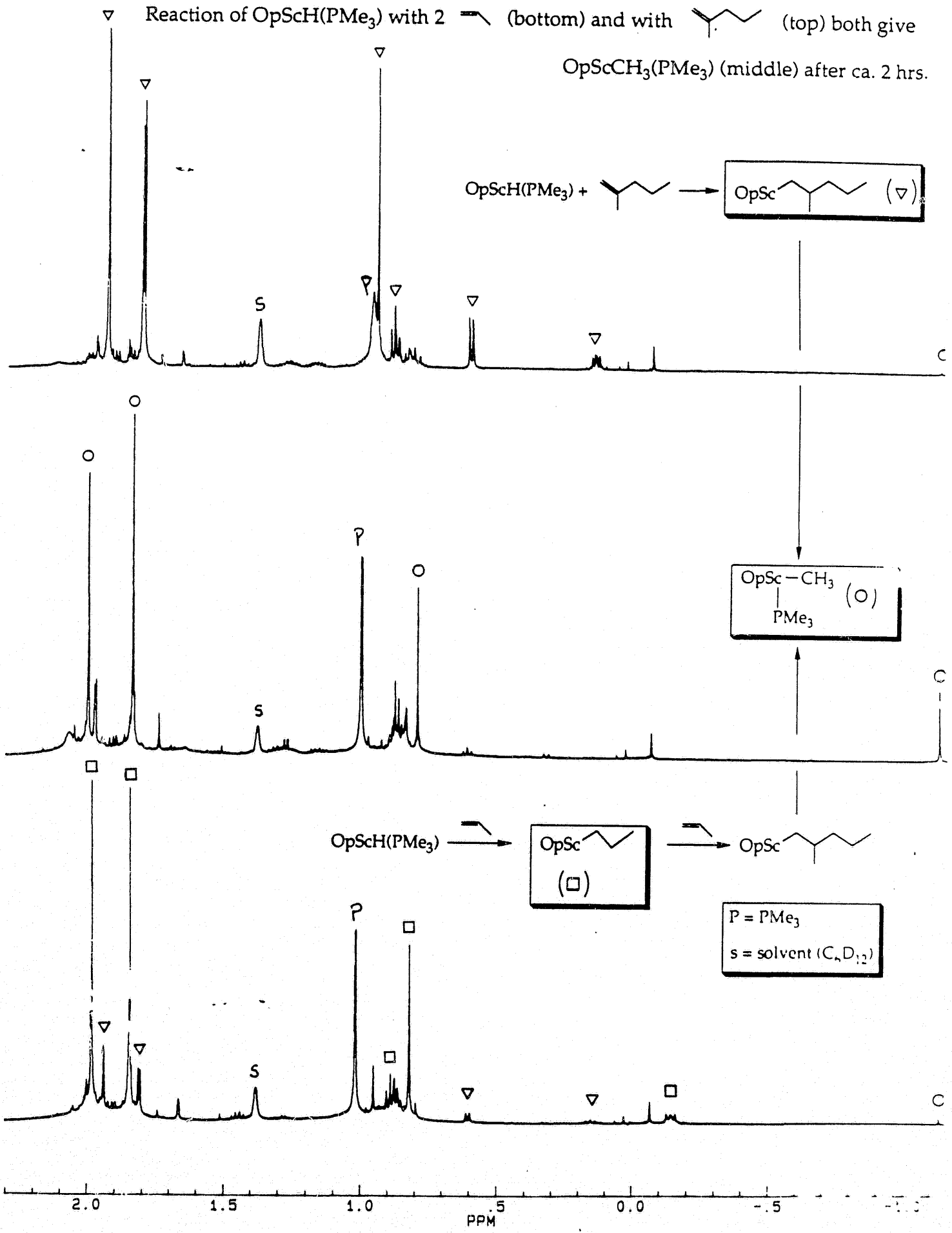


L-1154-M3

Reaction of $OpScCH_3(PMe_3)$ with propene

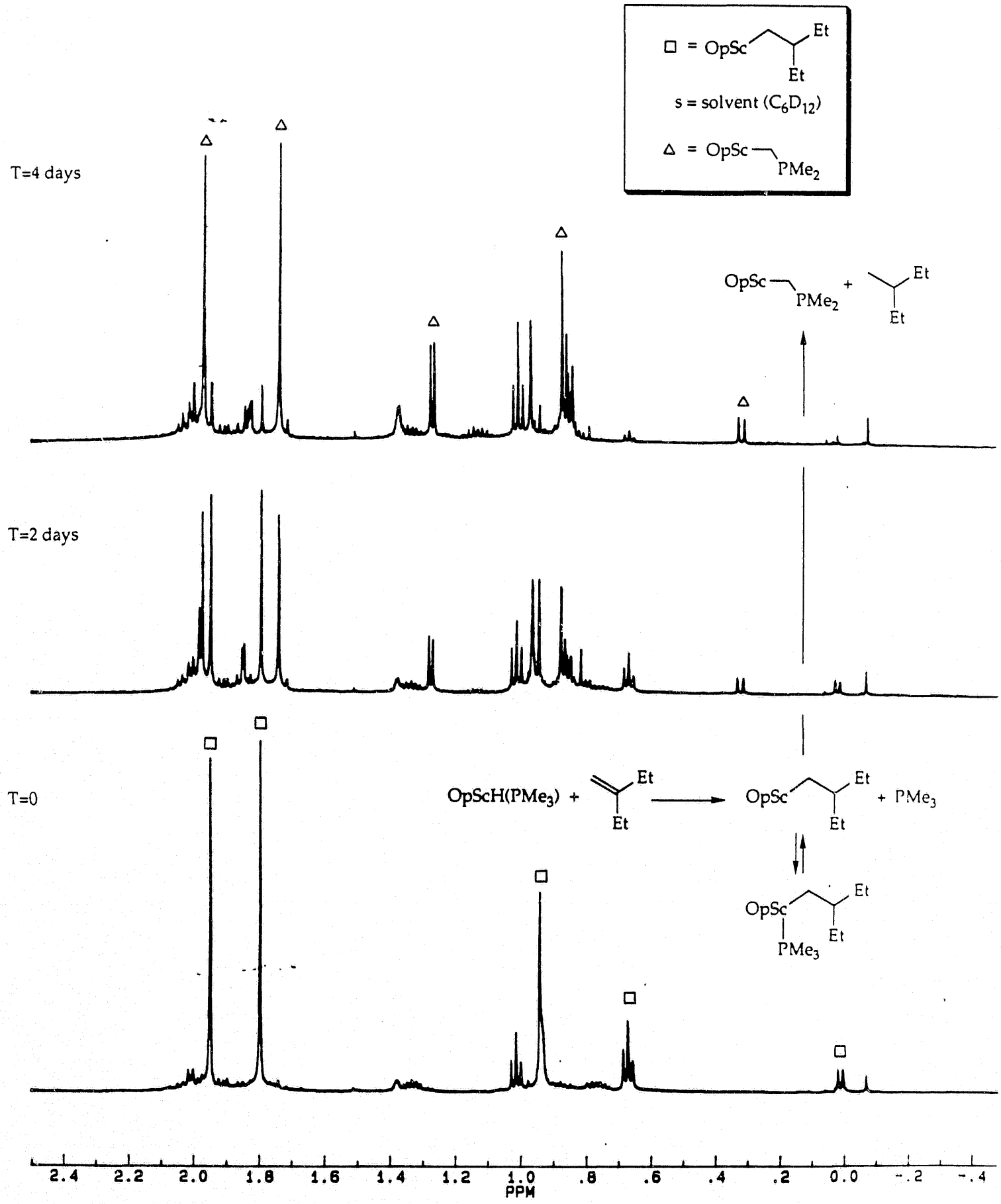


L-1154-M4


Reaction of OpScH(PMe3) with 2 (bottom) and with (top) both give
OpScCH3(PMe3) (middle) after ca. 2 hrs.
OpScH(PMe3) +
OpSc
(▽)
OpSc—CH3
PMe3
(○)
OpScH(PMe3)
OpSc
(□)
OpSc
P = PMe3
s = solvent (C6D12)
2.0
1.5
1.0
.5
0.0
-.5
PPM

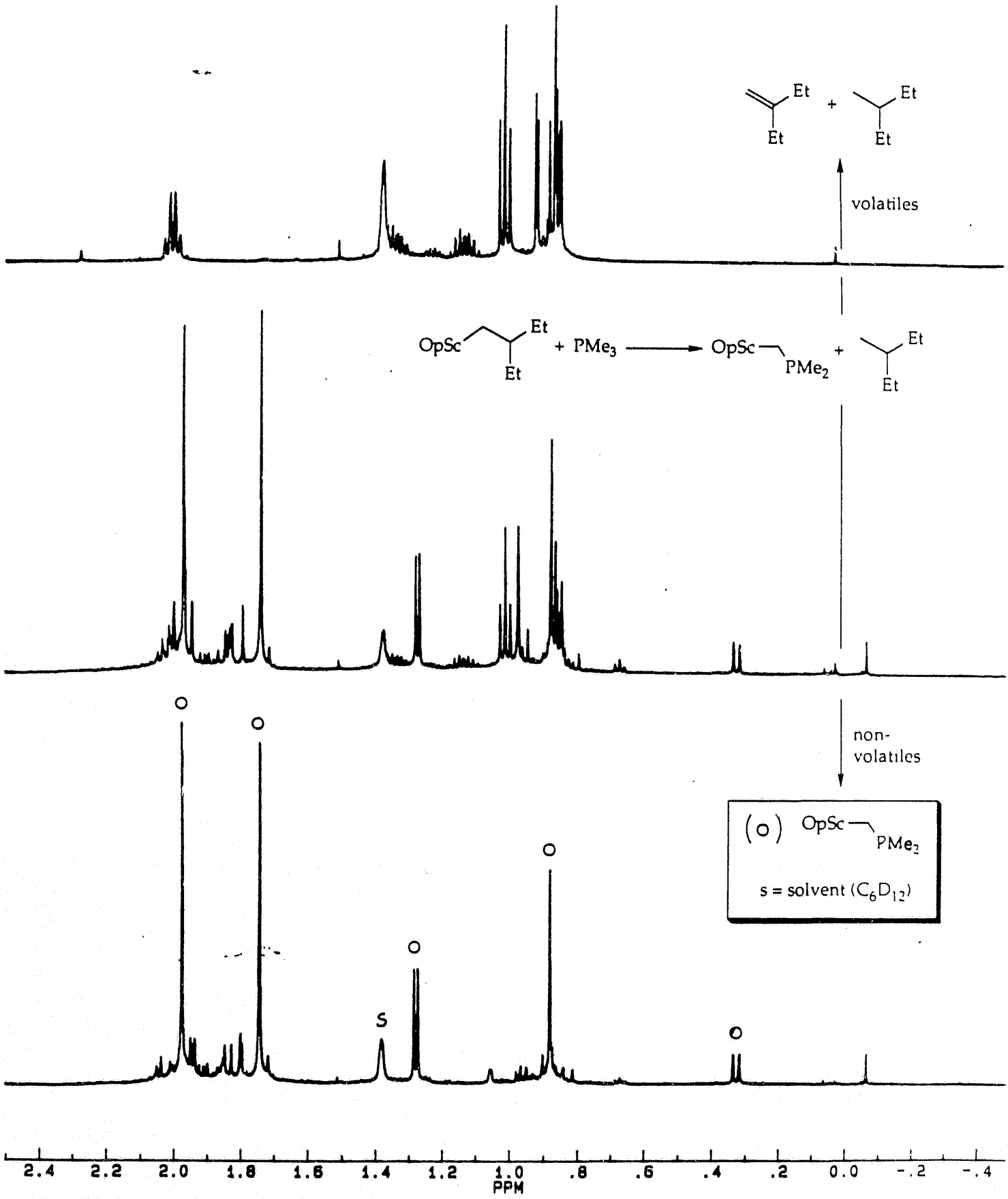
L-1154-M5

Rearrangement of OpSc(2-ethylbutyl) to $OpScCH_2PMe_2$

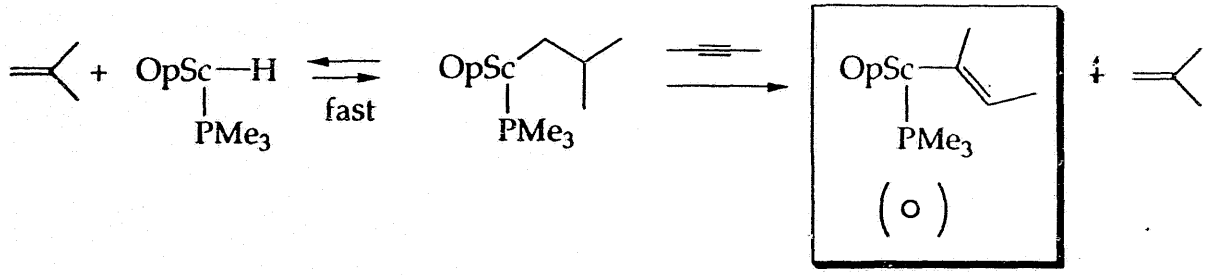


L-1154-M6

Characterization $OpScCH_2PMe_2$ by Pumping off Volatiles



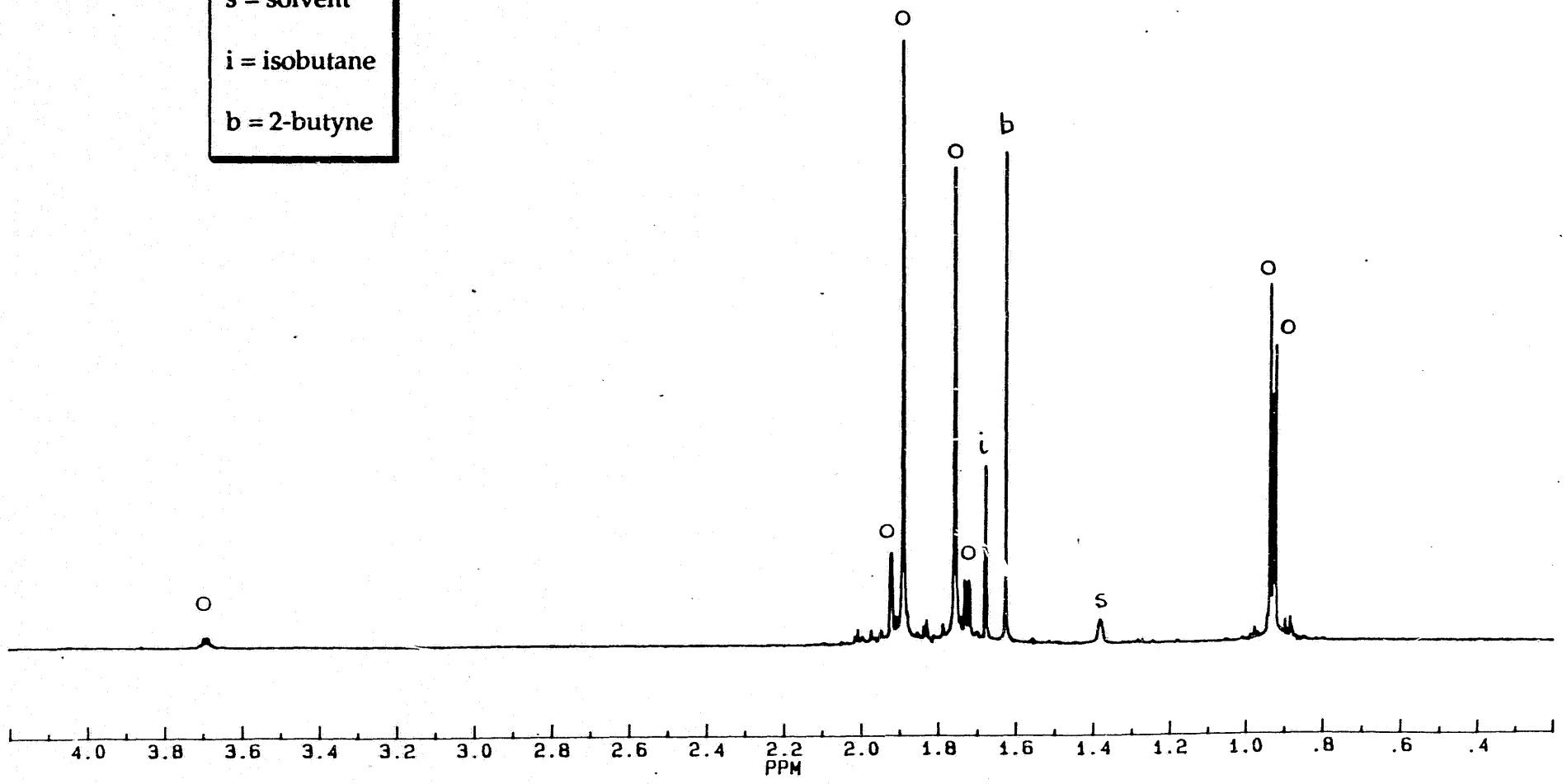
REACTION OF OPSC(ISOBUTYL) WITH EXCESS 2-BUTYNE



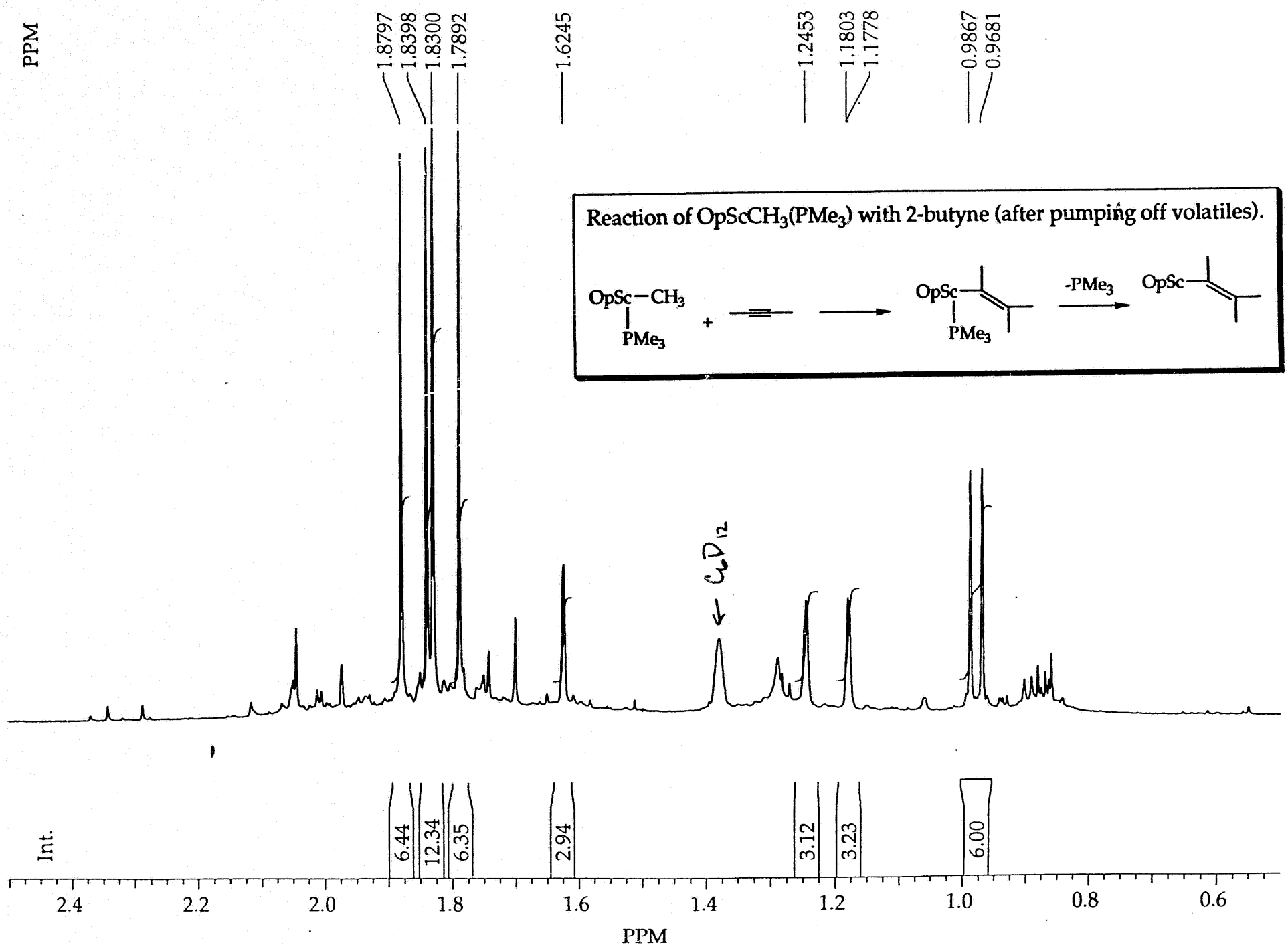
s = solvent

i = isobutane

b = 2-butyne



L-1524-79

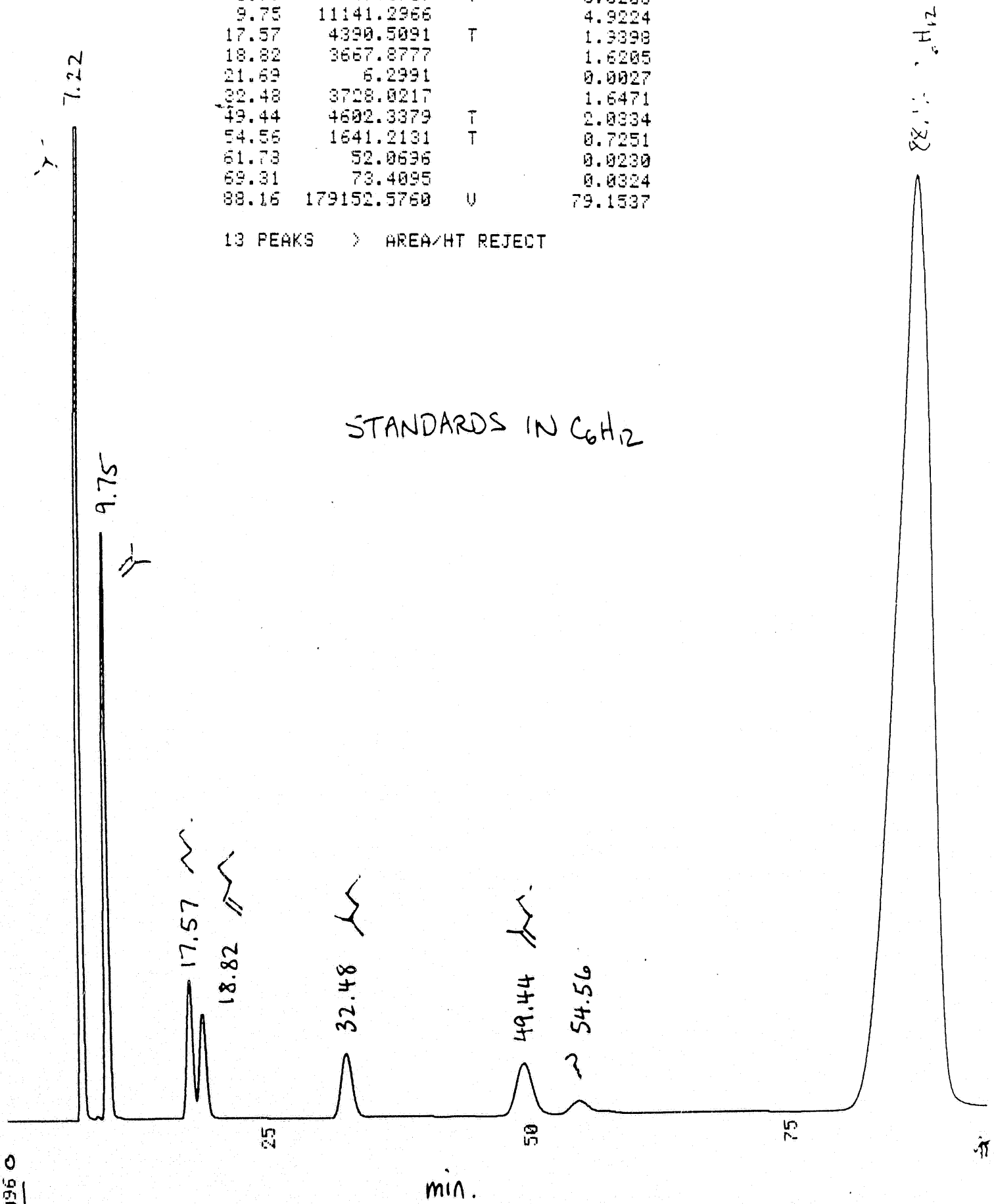

PPM
1.8797
1.8398
1.8300
1.7892
1.6245
1.2453
1.1803
1.1778
0.9867
0.9681
Reaction of OpScCH3(PMe3) with 2-butyne (after pumping off volatiles).
OpSc—CH3
PMe3
+
OpSc
PMe3
-PMe3
OpSc
C6D12
Int.
6.44
12.34
6.35
2.94
3.12
3.23
6.00
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
PPM

METHOD 1 MODIFIED CHROMATOGRAM

L-1154-M9

RT	AREA	BC	AREA %
5.88	1.7551		0.0007
7.22	17830.4768		7.8779
8.77	47.1707	V	0.0208
9.75	11141.2966		4.9224
17.57	4390.5091	T	1.9398
18.82	3667.8777		1.6205
21.69	6.2991		0.0027
32.48	3728.0217		1.6471
49.44	4602.3379	T	2.0334
54.56	1641.2131	T	0.7251
61.78	52.0696		0.0230
69.31	73.4095		0.0324
88.16	179152.5760	V	79.1537

13 PEAKS > AREA/HT REJECT



STANDARDS IN C_6H_{12}

4096 0

L-1154-M10

RUN 4 14:54 91/05/07

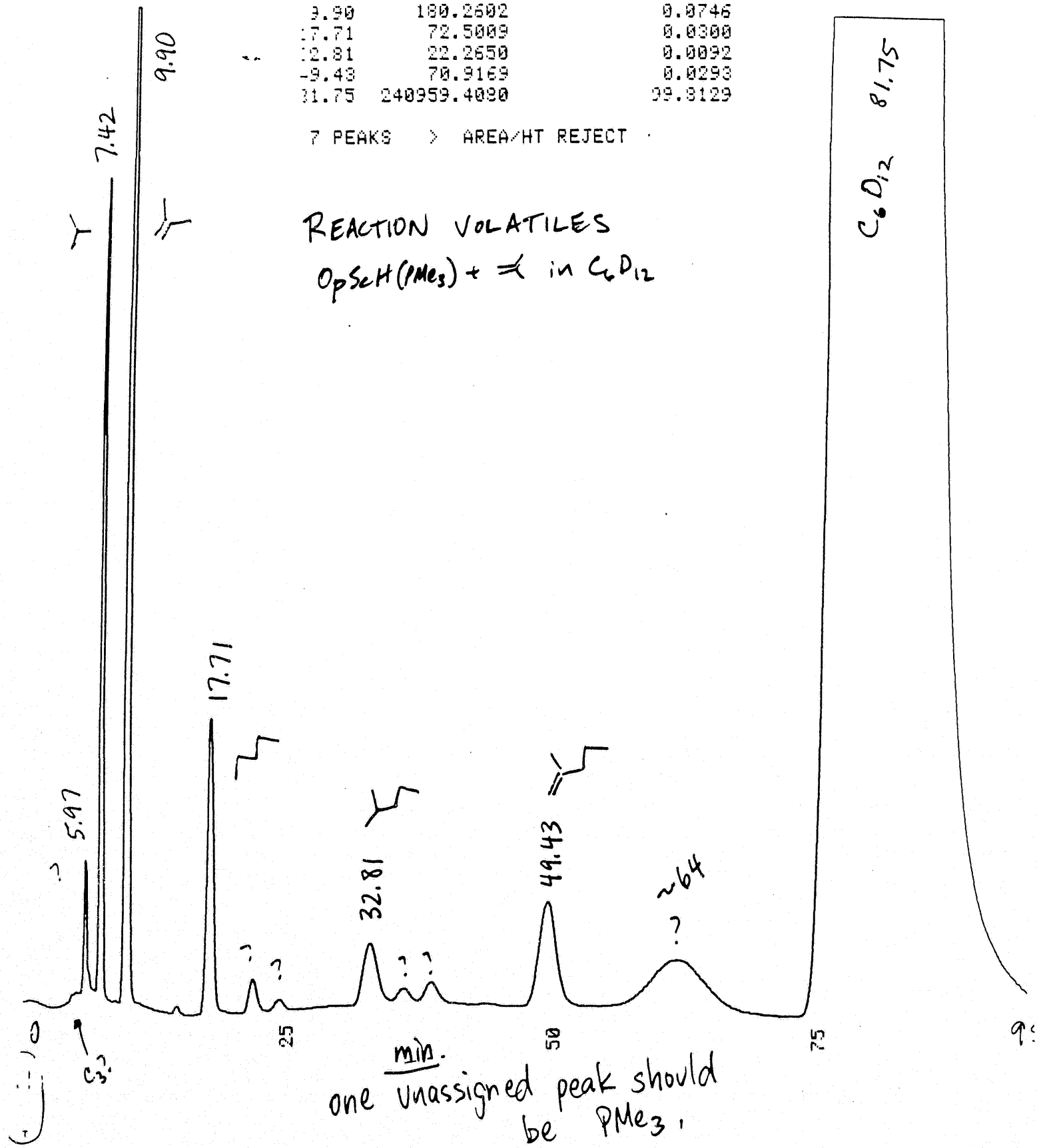
METHOD 1 MODIFIED CALCUL

RT	AREA	BC	AREA %
5.37	13.6453		0.0056
7.42	91.9962		0.0381
9.90	180.2602		0.0746
17.71	72.5009		0.0300
32.81	22.2650		0.0092
49.43	70.9169		0.0293
81.75	240359.4090		99.8129

7 PEAKS > AREA/HT REJECT

REACTION VOLATILES

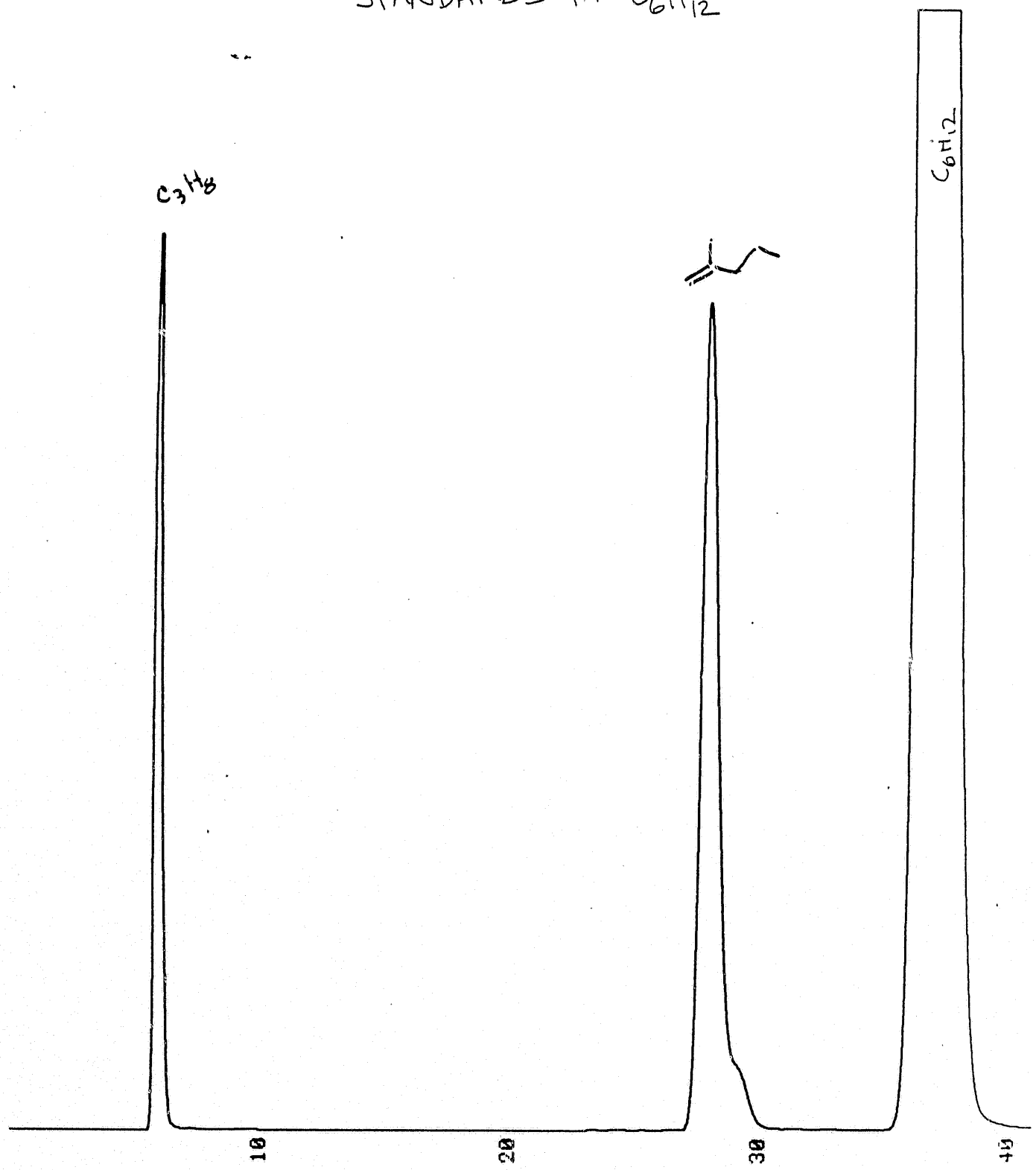
$Cp_2ScH(PMe_3)$ + ≠ in C_6D_{12}



one unassigned peak should be PMe_3.

L-1154-m11

STANDARDS in C_6H_{12}

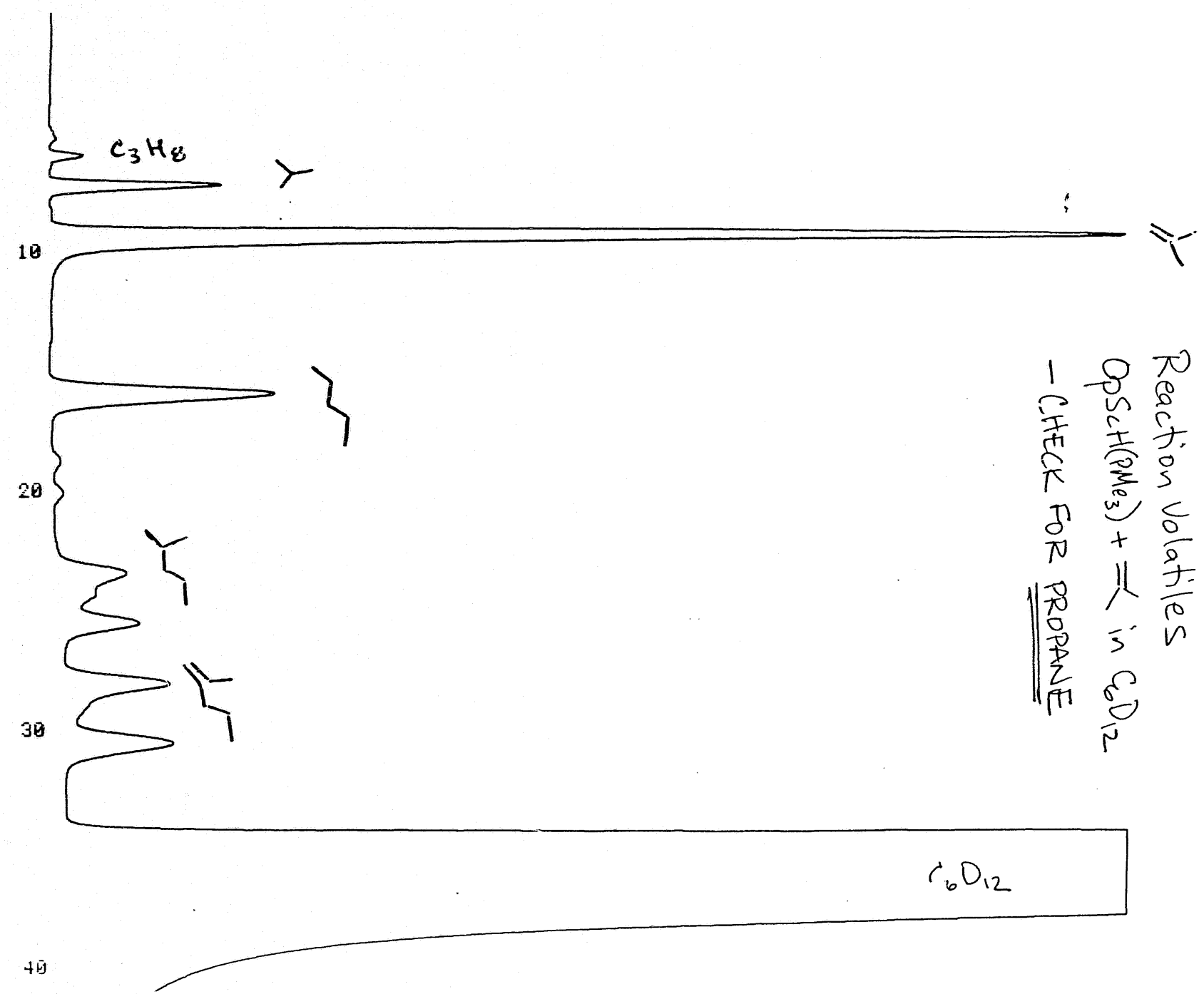


METHOD 3 MODIFIED

A 1024

RUN 11 4:53 93/04/20

METHOD 3 MODIFIED



Reaction Volatiles

$OpSCH(PMe_3) + =\!\!\!

L-1154-MB

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*LIST KINETIC.AU

------ FILE: KINETIC .AU

; ** KINETIC **

; PROGRAM TO ACQUIRE A SERIES OF EXPERIMENTS
; AT INTERVALS AND SAVE ON THE HARD DISK

; LDF/SPH 10TH MAY 1991


1    ZE                ; ZERO THE MEMORY
2    D1                ; RELAXATION DELAY

3    GO=2

4    WR #1             ; WRITE THIS EXPNT. TO DISK
5    IF #1             ; INCREMENT THE FILE EXTENSION

6    D2                ; DELAY BETWEEN EXPERIMENTS (SECONDS)
7    IN=1              ; LOOP BACK AND START THE NEXT EXPERIMENT

8    EXIT

; PW = PULSE WIDTH CA. 50 DEG.  4 US
; D1 = DELAY BETWEEN SCANS CA 2 SECS
; D2 = DELAY BETWEEN EXPERIMENTS (SECONDS)
; NS = NUMBER OF SCANS PER EXPERIMENT
; NE = NUMBER OF EXPERIMENTS
; RD = 0
```